201-16554J

IUCLID

Data Set

Existing Chemical	:	ID: 68515-50-4
Memo	:	HPV chemical
CAS No.	:	68515-50-4
TSCA Name	:	1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Generic name	:	dihexyl phthalate, branched and linear

Producer related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000

Substance related part

Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Status	:	
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	05.12.2006
Revision date	:	
Date of last update	:	05.12.2006
Number of pages	:	32
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Contact person	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

02.11.2001

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers: 68515-50-4, 71888-89-6, 27554-26-3, 68515-44-6, 111381-89-6 and 111381-90-9 (see remark for names)

Remark : This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers and names:

68515-50-4 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear (DHP)

71888-89-6 1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (DIHP)

27554-26-3 1,2,-benzenedicarboxylic acid, diisooctyl ester (DIOP)

68515-44-6 1,2-benzenedicarboxylic acid, diheptyl ester, branched and linear (DinHP)

111381-89-6 1,2-benzenedicarboxylic acid (C7, C9) ester, branched and linear (79P)

111381-90-9 1,2-benzenedicarboxylic acid, (C7,C11) ester, branched and linear (711P)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Transitional phthalates, are produced from alcohols with straight-chain carbon backbones of C4-6. Phthalate esters containing >10% C4-6 molecules were conservatively included in this subcategory. Six of the U.S. HPV chemicals, dihexyl (DHP), diheptyl, diisoheptyl, diisooctyl, heptyl nonyl (C7, C9) and heptyl undecyl (C7, C11) phthalates are included in this subcategory. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including dibutyl (DBP), butylbenzyl (BBP), and di(2-ethylhexyl) phthalate (DEHP). Data on a structurally similar material, di-n hexyl phthalate, was also included for read-across purposes.

Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP). Physicochemical properties also vary in that the lower molecular weight transitional phthalates are more water-soluble than higher transitional phthalates, but none would be considered to fall into the "high water soluble" category. What distinguishes these phthalates from others is their greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate subcategories. Of the phthalates in this subcategory, DEHP appears to be the most potent for liver and reproductive/developmental endpoints.

03.04.2006

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

02.11.2001

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Polymers industry
Remark	:	Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP).

02.11.2001

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	-27 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Remark	:	Data are from a peer reviewed literature review of data from a variety of sources including manufacturer's data or handbook values.
Test substance	:	CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Reliability	:	(2) valid with restrictions This robust summary is assigned a reliability of 2 because there is limited informtion on how the data were developed.
Flag	:	Critical study for SIDS endpoint

05.12.2006 (12)

Value	:	49 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculation
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Method	:	Melting point calculation by MPBPWIN ver. 1.41 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation. However, the melting point calculation in EPI SuiteTM gives erroneously high results for the phthalate esters.
Test substance	:	CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Reliability	:	(3) invalid

03.04.2006 (4)

2.2 BOILING POINT

Value	:	373 °C at 1013 hPa
Decomposition	:	
Method	:	other: calculation
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Method	:	Boiling point calculation by MPBPWIN ver. 1.41 using calculation method of Stein and Brown.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Reliability	:	(2) valid with restrictions

This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
05.07.2006 (4)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .00000344 hPa at 25 °C
Decomposition : no
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Method : Measured data collected and tabulated, calculated data also considered in determining recommended values.

Remark : Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for vapour pressure, represent the definitive and currently accepted physicochemical database for selected phthalate esters including dihexyl (branched and linear) phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for dihexyl (branched and linear) phthalate ester was 431.6 cm3 mol-1.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r2 = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r2 = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r2 = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
03.04.2006 (2)

Value	:	.0000301 hPa at 25 °C
Decomposition	:	no
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.41 using calculation method of Grain.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

03.04.2006 (4)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	6 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for partition coefficient, represent the definitive and currently accepted physicochemical database for selected phthalate esters including dihexyl (branched and linear) phthalate. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for dihexyl (branched and linear) phthalate ester was 431.6 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41 It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.
Test substance	:	CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched

and linear

Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint

05.07.2006 (2)

Partition coefficient : octanol-water
Log pow : 6.46 at 25 °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Method : Partition coefficient by LOGKOWWIN ver. 1.67 using an atom/fragment calculation method of Meylan and Howard.
Remark : EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance : CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

03.04.2006 (4)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : .159 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year :
GLP :
Test substance : other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Method : Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark : Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for water solubility, represent the definitive and currently accepted physicochemical database for selected phthalate esters including dihexyl (branched and linear) phthalate.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume

(cm3 mol-1). The Le Bas molar volume used for dihexyl (branched and linear) phthalate ester was 431.6 cm3 mol-1.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r2 = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r2 = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r2 = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint

03.04.2006 (2)

Solubility in : Water
Value : .023 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year :
GLP :
Test substance : other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Method : Water solubility calculated using WSKOWN ver 1.41 based on Kow correlation method of Meylan and Howard. Kow used in calculation was 6.46.

Remark : EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.

Test substance : CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

03.04.2006 (4)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	1 based on intensity of sunlight
Conc. of substance	:	at 25 °C
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	.00000000001129 cm³/(molecule*sec)
Degradation	:	50 % after 11.4 hour(s)
Deg. product	:	not measured
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.91 based on the methods of Atkinson.
Remark	:	50% degradation after 11.36 hrs or 0.947 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration. EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag	:	Critical study for SIDS endpoint

05.07.2006 (4)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	3.5 year at 25 °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.
Flag : Critical study for SIDS endpoint
12.05.2006 (4)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : other: air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	334.46
Temperature	25° C
Log Kow	6.0
Water Solubility	0.159 g/m3
Vapor Pressure	0.000344 Pa
Melting Point	-27°C

Result : Using the Mackay Level I calculation, the following distribution is predicted for 1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear:

% Distribution	Compartment
0.0	Air
0.1	Water
97.6	Soil
2.2	Sediment
0.1	Suspended Sediment
0.0	Biota

Test substance : CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.
Flag : Critical study for SIDS endpoint
03.04.2006 (8)

Media : other: air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	334.46
Temperature	25° C
Log Kow	6.0
Water Solubilit	0.159 g/m3
Vapor Pressure	0.000344 Pa
Melting Point	-27°C

Emissions rates used in the calculation:

Compartment	Rate (kg/hr)
Air	1000
Water	1000
Soil	1000

Half-lives used in the calculation:

Compartment	Half-life (hr)
Air	22.7a
Water	120b
Soil	420c
Sediment	420c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI SuiteTM version 3.12 and normalized to a 24 hour day [Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on biodegradation data from: Exxon Biomedical Sciences, Inc. Ready Biodegradability: Manometric Respirometry Test, Study Number 142994A, 1997 Exxon Biomedical Sciences, Inc.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Result : Using the Mackay Level III calculation, the following distribution is predicted for 1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear:

Compartment	% Distribution
Air	2.1
Water	12.3
Soil	72.2
Sediment	13.4

Test substance : CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
12.05.2006

(8)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type	:	aerobic
Inoculum	:	activated sludge
Concentration	:	36.39 mg/l related to Test substance related to
Contact time	:	
Degradation	:	= 79.7 (±) % after 28 day(s)
Result	:	readily biodegradable
Control substance	:	other
Kinetic	:	% %
Deg. product	:	
Method	:	OECD Guide-line 301 F "Ready Biodegradability: Manometric Respirometry Test"
Year	:	1983
GLP	:	no
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Method	:	OECD 301F, Ready Biodegradability, Manometric Respirometry Test
Result	:	Test material was readily biodegradable. Half-life was <2 weeks. By day 28, 79.7% degradation of the test material was observed. 10% biodegradation was achieved on approximately day 6, 50% biodegradation on approximately day 10. By day 14, >60% biodegradation of positive control was observed, which meets the guideline requirement. No excursions from the protocol were noted. Biodegradation was based on oxygen consumption and the theoretical oxygen demand of the test material as calculated using results of an elemental analysis of the test material.

Sample	% Degradation* (day 28)	Mean % Degradation (day 28)
n-Pentane	87.9, 82.6, 68.5	79.7
Na Benzoate	95.9, 92.4	94.2

* replicate data

Interval results for the test substance are as follows:

Day	% Degradation (mean of tripicate systems)
6	7.0
7	20.9
10	55.6
14	66.8
21	77.2
28	79.7

Test condition	:	Treatment replicates were prepared by combining glass-distilled water, a mineral substrate, pH buffer, activated sludge and the appropriate test substance. Three replicates of the test material and two replicates of positive control (sodium benzoate) were prepared and evaluated in 1L glass vessels. Oxygen consumed by microorganisms from the oxidation of the test

substance was continuously monitored by an automatic respirometer.

Test flasks were continuously stirred for 28 days. Test temperature was 22 +/- 1 Deg C.
Concentration-Nominal test concentration = 36 to 39mg/L for test substance.
Nominal concentration of the positive control (sodium benzoate) was 51 mg/L

Test substance : Dihexyl Phthalate (CAS# 68515-50-4)
(1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear)
Synonym: DHP
No information on purity.

Conclusion : The substance is readily biodegradable.

Reliability : (2) valid with restrictions
The study was conducted according to guidline with an audit of the data, but under a GLP protocol.

Flag : Critical study for SIDS endpoint

27.04.2006 (6)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	flow through
Species	:	Oncorhynchus mykiss (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
LC50	:	>= .2 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	other
Year	:	1975
GLP	:	yes
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Method : Method/Guideline-USEPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, 1975. Macroinvertebrates, and Amphibians.

Statistical methods-Moving average angle, Probit or Bionomial concentration.

Result : 96 hr LC50 >0.20 mg/L
Mean measured values were used in the LC50 calculation.

Nominal test concentrations: control, 0.018, 0.036, 0.072, 0.14, and 0.29 mg/L.
Mean measured test concentrations: <0.0042, 0.014, 0.040, 0.057, 0.093, and 0.20 mg/L.

Analytical samples were taken at time zero and on a composite of replicates at study termination. Measured values dropped slightly during the exposure period. One replicate of the second highest concentration exhibited mortality and may have been due to physical effects rather than toxicity.

% Mortality results at 96 hrs per replicate for control and treatment levels:

Conc. (mg/L)	Rep1/Rep2
Control	0 / 0
0.014	0 / 0
0.040	0 / 0
0.057	0 / 0
0.093	0 / 10
0.20	0 / 0

Test condition : Test treatments were prepared by using a proportional diluter modified to enhance mixing of phthalates. The dilution water was Wareham Mass. town water (untreated and unchlorinated). A concentrated stock solution was prepared and combined with dilution water prior to pumping into the diluter. The diluter delivered a series of stock dilutions to the test vessels. Test chambers were glass tanks containing 15 L of solution. The diluter maintained a water turnover rate of 5 to 8 tank volumes per day. Two replicates of ten organisms were tested per treatment and control. Analytical method was Gas Liquid Chromatography (GLC) with electron capture detection.

Fish mean length = 62 mm and mean wet weight = 2.3 g. Test temperature = 12 Deg C. The pH ranged from 7.2 to 7.5. The mean dissolved oxygen ranged from 9.2 to 9.4 mg/L. Ranges of total hardness and alkalinity as CaCO3 of the dilution water were 20 to 26 mg/L and 14 to 22 mg/L, respectively.

Fish were obtained from a Montana supplier.

Test substance : Dihexyl phthalate (CAS# 68515-50-4)
(1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear)
Synonym: DHP
Purity: 100% active ingredient

Conclusion : Test substance is non-toxic to fish at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).

Reliability : (1) valid without restriction
This summary is rated a "1" and represents a key study because it followed an U.S. EPA standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.

Flag : Critical study for SIDS endpoint
27.04.2006 (3) (13)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
EC50 : > .18 measured/nominal
Analytical monitoring : yes
Method : other
Year : 1975
GLP : yes
Test substance : other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Method : Method/Guideline - U.S. EPA, (660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. 1975.

Statistical methods - Moving average angle, Probit or Bionomial Concentration.

Result : 48 hr EC50 >0.35 mg/L (based upon time zero analytical samples; no effects at test substance saturation). Value was recalculated as >0.18 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997).

Mean measured values were used in the final EC50 calculation.

Nominal test concentrations: control, 0.052, 0.086, 0.14, 0.24, and 0.40 mg/L.
Mean measured test concentrations of time 0 and 48 hr values: <0.0083, 0.019, 0.028, 0.059, 0.104 and 0.18 mg/L.

Analytical samples taken at time zero and on a composite of replicates at termination. Measured values declined to a level at or below the detection limit during study exposure. The high treatment solution is considered the maximum solubility achievable under the conditions of the test.

% Immobility results at 48 hrs per replicate for control and treatment levels in the first test:

Conc. (mg/L)	Rep1/Rep2/Rep3
Control	0 / 0 / 20
0.019	0 / 0 / 0

0.028	0 / 0 / 20
0.059	20 / 20 / 20
0.104	0 / 20 / 20
0.18	0 / 20 / 20

% Immobility results at 48 hrs per replicate for control and treatment levels in the second limit test performed to confirm the results of the first study:

Conc. (mg/L)	Rep1/Rep2/Rep3
Control	0 / 0 / 0
0.056	0 / 0 / 10

Nominal test concentrations: control and 0.22 mg/L.
Mean measured test concentrations of time 0 and 48 hr values: <0.0080 and 0.056 mg/L.

Water quality information for the second test was limited.

Data from the first test are used to characterize the acute toxicity of the test substance.

Test condition : Test treatments were prepared by mixing the test substance and dilution water (fortified well water) in a Polytron homogenizer for 30 minutes. The stock solution was prepared at the highest treatment concentration. Dilutions of the stock were prepared for each treatment level. Three replicates of five organisms were tested per treatment. Test vessels were 250 ml beakers with 200 ml of test solution. Analytical method was Gas Liquid Chromatography (GLC).

Water quality parameters for the first test:
Test temperature = 22.5 +/- 0.5 Deg C. The pH ranged from 8.3 to 8.6 at initiation and was 8.3 in the control and all exposure solution on day 2. Dissolved oxygen ranged from 7.0 to 8.7 at initiation and 7.3 to 8.4 on day 2. The range of total hardness of the dilution water was 150 to 170 mg/L. Daphnia were <24 hours old and obtained from in-house stock.

Water quality parameters for the second test:
The range of total hardness of the dilution water was 150 to 170 mg/L. Daphnia were <24 hours old and obtained from in-house stock.

Test substance : Dihexyl phthalate (CAS# 68515-50-4)
(1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear)
Synonym: DHP
Purity: unstated, but believed to be 100% active ingredient because the test material came from the same source as in the rainbow trout acute study.

Conclusion : Test substance is non-toxic to Daphnia at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).

Reliability : (2) valid with restrictions
Loss of measureable test substance during exposure.

Flag : Critical study for SIDS endpoint

27.04.2006 (10) (13)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint :
Exposure period : 7 day(s)
Unit : mg/l
NOEC : = .33

EC50	:	> .33 measured/nominal
Limit test	:	
Analytical monitoring	:	yes
Method	:	other
Year	:	1978
GLP	:	yes
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Method : Method/Guideline - EPA 600/9-78-018, Printz Algal Assay Bottle Test. 1978.
Statistical methods - Moving average angle, Probit or Bionomial
Test type - Static

Result : 168 hr (7 day) EC50 >0.6 mg/L (based upon time zero analytical samples). Value was recalculated as >0.33 mg/L as per U.S. EPA current practices using mean of measured initiation and termination samples as reported in Staples et al. (1997).

Mean measured values were used in the final EC50 calculation.

Nominal test concentrations as a percent of a saturated solution: 0 (control), 3.125, 6.25, 12.5, 25.0, 50.0 and 100.0%.
Mean measured test concentrations of time 0 and 168 hr values: <0.10, 0.10, <0.10, 0.10, 0.10, 0.20, and 0.33 mg/L (detection limit was 0.1 mg/L).

Analytical samples taken at time zero and on a composite of replicates at termination. In-vivo chlorophyll a, measured until less than 5% change. Both cell number and in-vivo chlorophyll a, measured at termination. Control chlorophyll a or cell counts were not reported. A stimulatory effect as compared with the control was measured in the lowest two test concentrations throughout the 7-day exposure period except for day 5, which showed only slight decreases. Cell number on day 7 in these two treatments also exhibited an increase of 9 and 10% relative to the control. After 7 days of exposure, the percent change in relative fluorescence units was positive relative to the control in all but the highest treatment level and ranged from +3 to +8% in the 4 low treatment levels. The highest treatment level exhibited a -18% on day 7. After 7 days exposure, the percent change in cell number in treatments relative to the control ranged from +19% in an intermediate treatment level concentration to -23% in the highest concentration. Confidence limits could not be calculated since the percent change did not exceed 25% on day 7. Analytical samples were taken at time zero and on a composite of replicates at termination.

Chlorophyll a percent change relative to control on sampling days and cell number on day 7 results per treatment level:

Conc. (mg/L)	Chlorophyll a percent change from control Day 3	Day 5	Day 6	Day 7	Cell # Day 7
0.1	+14	-4	+3	+3	+9
<0.1	0	-2	+5	+8	+10
0.1	+4	-12	0	+3	-7
0.1	-25	-18	-17	+6	+19
0.2	-59	-29	-16	+6	-2
0.33	-66	-49	-36	-18	-23

Test condition : Test substance was added to Algal Growth Medium equal to the highest test concentration (1000 mg/L) and stirred for one hour and settled for one-half hour. Fifty percent (50%) dilutions were made of this stock solution using algal growth media (dilution water and control) and tested. Initial algal concentration was 2.0 E4 cells/ml. Replicate number was not cited.

Lighting = 4,500 lux, Test temperature = 24+/-1 Deg C. The pH range was 7.4 to 7.5 at initiation and 7.0 to 7.5 on day 7. Algal culture stock was

obtained from University of Texas at Austin, TX.

Test substance	:	Dihexyl Phthalate (CAS# 68515-50-4) (1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear) Synonym: DHP Purity: unstated, but believed to be 100% active ingredient as was provided in the rainbow trout study.
Conclusion	:	Test substance is not toxic to algae at or below its water solubility level. Data selected based upon routine species, measured data and representative value, as compared with those found in reference document, Staples et al. (1997).
Reliability	:	(1) valid without restriction Control and exposure chlorophyll a or cell counts not reported.
Flag	:	Critical study for SIDS endpoint

27.04.2006 (11) (13)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

Species	:	Oncorhynchus mykiss (Fish, fresh water)
Endpoint	:	other: Early Life Stage Toxicity Test
Exposure period	:	111 day(s)
Unit	:	mg/l
NOEC	:	= .22 measured/nominal
Analytical monitoring	:	yes
Method	:	other
Year	:	
GLP	:	yes
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Method	:	Testing procedures followed the US Environmental Protection Agency, Toxic Substance Control Act (EPA-TSCA) 40 CFR, Part 797.1600 as modified in Testing Consent Agreement 40 CFR, Part 799 (1989), and the American Society for Testing and Materials (ASTM) Standard Guide for Conducting Early Life-Stage Toxicity Tests with Fishes (1990).
Result	:	Egg hatchability/survival, fry survival, and growth (length and weight) were evaluated as the biological endpoints. Dihexyl phthalate ester showed no effect on hatchability, survival, or growth at its highest achievable water solubility (0.22 mg/L) under the conditions of this test. Mean standard fish length (mm): Control replicates = 99.4 +/- 7.4 Treatment replicates = 95.5 +/- 6.7 to 101.6 +/- 7.3 Pooled treatment replicates (n=70) = 99.0 +/- 7.8 Mean standard fish weight (g): Control replicates = 18.08 +/- 4.75 Treatment replicates = 16.18 +/- 3.84 to 19.46 +/- 5.0 Pooled treatment replicates (n=70) = 18.01 +/- 4.93 The study was terminated 9 days prior to the planned 120-day post-hatch exposure period due to a mechanical failure of the proportional diluter system. This malfunction, interrupting water flow to all control and expousre aquaria, resulted in a significant decrease in dissolved oxygen concentrations. As a direct result substantial mortality occurred throughout all test aquaria. Consequently, the results represent a 111-day post hatch exposure (143 days total exposure). Significant mortality occurred as

quickly as 2 hours after mechanical failure because at that point in the study, the fish are large enough that even a brief interruption in water flow results in severe oxygen depletion and asphyxiation. The results up to the interruption are reported as it was determined that the study results were not compromised by the early termination.

Test condition : The study used a flow-through test system. Test substance exposure solutions were prepared by mixing an appropriate amount of test substance into acetone (carrier solvent) to form a diluter stock solution. Control systems received an amount of carrier solvent approximately equivalent to the highest exposure concentration. The diluter stock solution was metered into a diluter chemcial mixing cell with a syringe injector. A sonicator was incorporated into mixing cell that received stock solution from the proportional diluter. Exposure solution then flowed to the test systems.

In the high exposures, small droplets of test substance formed, which were physically removed by skimming the medium surface during the diluter cycle. No visible film was seen on the surface of exposure systems.

At study initiation, 40 to 60 Oncorhynchus mykiss embryos were impartially distributed into smaller incubation chambers that were suspended in each test system. The incubation chambers were mechanically oscillated vertically in each test system by a rocker arm to facilitate test solution circulation and to keep the embryos clean.

On day 25, embryos were impartially reduced to 20 eyed embryos in each chamber. After hatch (35 days post fertilization) sac-fry were released from the incubation chambers into the test system. Developing embryos were maintained under low light through hatch. After hatch, a 14:10 hour light:dark photoperid with a simulated dawn and dush transition period was maintained. Light intensity over the test systems during the day photoperiod was approximately 50 lumens/ft2.

Beginning at the start of swim-up, fish were fed a comercially prepared Salmon Starter® (Zeigler Bros, Gardners, PA, USA) in combination with live brine shrimp mauplii (Artemia sp.). Fish were fed two to three times a day. Test systems were siphoned daily during the growth phase to remove fecal material and uneaten food and to minimize microbial growth.

The total exposure time was 143 days, 111 days post-hatch.

At test termination, standard length of fish was determined photographically, after which fish were sacrificed and measured again for length and dry-blotted wet weight.

Water quality measurements were determined periodically during the tests in one or more replicates at intervals ranging from once daily to once weekly. Test conditions during incubation and growth were:

Temperature = 10 +/- 1.5 degree C during egg incubation
Temperature = 12 +/- 1.5 degree C during growth phase
Water harness = 158 to 180 mg/L (as CaCO3) in control and treatments
Alkalinity = 182 to 204 mg/L (as CaCO3) in control and treatments
pH = 7.7 to 8.6 in control and treatments
Dissolved oxygen = 8.8 mg/L in control replicates
Dissolved oxygen = 8.0 to 8.6 mg/L in treatment replicates
(Dissolved oxygen in control and treatment replicates represent 78 to 85% of saturation.)

Test substance analyses of exposure solutions were performed using gas chromatography. The mean measured test substance concentrations were: 0.014, 0.029, 0.058, 0.10, and 0.22 mg/L, which represented 100, 104, 105, 91, and 100% of the nominal test concentrations of 0.014, 0.028,

0.055, 0.11, and 0.22 mg/L.

Test substance : The test was conducted using a uniformly ring-labeled 14C-dihexyl phthalate ester.

Conclusion : The chronic fish (Oncorhynchus mykiss) toxicity (early life-stage) data reported for dihexyl phthalate are consistent with the data for several high molecular weight phthalate esters as summarized by Rhodes et al. (1995). These data clearly showed that high molecular weight phthalate esters, including dihexyl phthalate, did not produce chronic toxicity to a fish at or below their maximum attainable water solubility.

Reliability : (1) valid without restriction
This study is rated a "1" because it followed an accepted test guideline, used appropriate testing procedures, and applied GLP. The study procedure and results were accepted in a peer reviewed journal. Additionally, the data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances.

Flag : Critical study for SIDS endpoint
27.04.2006 (1) (9)

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	13 weeks (90 days)
Frequency of treatm.	:	Daily for 13 weeks
Post exposure period	:	None
Doses	:	0, 0.05%, 0.1% and 0.5% (the 0.05% group was adjusted to 1.0% at 7 weeks and 3.0% at 12 weeks)
Control group	:	yes
NOAEL	:	= .5 %
LOAEL	:	= 3 %
Method	:	other
Year	:	1962
GLP	:	no
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Method	:	ANOVA; homogeneity of variance tested by method of Bartlett; differences from control y methods of Scheffe or Fischer-Behrens (modified t-test) Control Group: 10/sex/dose
Remark	:	Rats in the 0.05% group, which was increased to 1.0% at 7 weeks and 3.0% at 12 weeks displayed signs of respiratory distress, stiff gait, and rigidly or arched tail over the last three weeks of the study. Body weight gains and food consumption also were decreased for this group over that period. Total leukocyte counts were significantly increased for the 3.0% females at 90 days; blood chemistry, hematology and urinalysis values were comparable for all other groups and intervals. Heart/body weight

ratios for males in all three dose groups and thyroid weights for females in the 0.1% group were significantly increased over the controls. Rats of both sexes in the 3.0% group showed significantly increased liver weights and decreased spleen, kidneys, adrenals, and gonads weights. Microscopic examination tissues from rats in the 3.0% group revealed atrophy of the spermatogenic epithelium in the testes and slight changes in the liver characterized as eosinophilic areas in the cytoplasm and variation in the size of the nuclei.

Result : The NOAEL was 0.5% in the diet (approximately 383 mg/kg/day). The LOAEL was approximately 5.0%.

Test condition : Male and female rats were fed the test substance daily for 13 weeks at dietary levels of 0, 0.05%, 0.1% and 0.5%. The 0.5% group was increased to 1.0% at 7 weeks and 3.0% at 12 weeks. Clinical observations, body weights and food consumption were recorded weekly. Clinical blood chemistry, hematology, and urinalysis were performed on 5 rats/sex/group at 30 and 90 days. A complete necropsy was performed after 13 weeks and organ weights were recorded. Tissues from the control, 0.5% and 3.0% groups were examined microscopically.

Test substance : 1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear (disohexyl phthalate) containing no more than 15% diheptyl phthalate.

Conclusion : Significant effects were found only at the highest dose tested (3%).

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint

05.07.2006 (5)

Type :
Species : dog
Sex : male/female
Strain : Beagle
Route of admin. : oral feed
Exposure period : 13 weeks (90 days)
Frequency of treatm. : Daily
Post exposure period : None
Doses : 0, 0.1, 0.5, or 1.0% (low dose adjusted to 5.0% during weeks 9-13)
Control group : yes
NOAEL : = 1 %
LOAEL : = 5 - %
Method : other
Year : 1962
GLP : no
Test substance : other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear

Remark : All animals appeared normal in appearance and behavior throughout the study. No significant variations in weight were attributed to the test substance. Clinical blood chemistry, hematology, and urinalysis values were within normal limits and comparable to the controls, Mean liver weights and liver/body weight ratios for the dogs in the 5.0% group increased, and the males also exhibited decreased testes weight and ratio. Enlarged hepatic cells were observed in the males in the 5.0% group; these two males also exhibited atrophy of the seminiferous epithelium in the testes.

Result : The NOAEL was 1.0% (approximately 180 mg/kg/day).

Test condition : Male and female beagle dogs were fed the test substance daily for 13 weeks at dietary levels of 0.1, 0.5, or 1.0% (the 0.1% level was increased to 5.0% at week 9). The animals were observed daily; body weights and food consumption were recorded weekly. Hematology, blood chemistry, and urinalysis were performed initially and at 30 and 90 days. A complete necropsy was performed after 13 weeks. Organ weights were recorded and the tissues from the control and high dose groups were examined microscopically.

Test substance : 1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear

(diisohexyl phthalate)

Conclusion	:	Significant effects were found only at the highest dose tested (5%).
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

05.07.2006 (5)

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Micronucleus assay
Species	:	mouse
Sex	:	male/female
Strain	:	CD-1
Route of admin.	:	gavage
Exposure period	:	Single dose with sacrifices at 24, 48 and 72 hours
Doses	:	0, 1250, 2500, and 5000 mg/kg
Result	:	negative
Method	:	OECD Guide-line 474 "Genetic Toxicology: Micronucleus Test"
Year	:	1994
GLP	:	yes
Test substance	:	other TS: CAS #68515-50-4; 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear
Method	:	Three groups of 5/sex/dose served as vehicle controls (corn oil) for the 24, 48, and 72 hour sacrifices; a single group of 5/sex/dose served as the positive control (cyclophosphamide) and was sacrificed at 24 hours. Statistical Methods: Analysis of variance (ANOVA) on proportion of cells with micronuclei per animal; Tukey's Studentized range test to determine which dose groups were different from the control.
Remark	:	The test substance induced no significant increases in micronucleated polychromatic erythrocytes over the levels observed in the concurrent vehicle control groups in eigher sex or at any sacrifice interval. The positive control group exhibited significant increases in both sexes.
Test condition	:	The test substance was solubilized in corn oil and dosed at a volume of 10 ml/kg. A total of 130 mice were used in the study; 15 sex/dose with 5/sex/dose sacrificed at 24, 48, or 72 hours after dosing. Bone marrow smears were prepared and stained after sacrifice. 1000 polychromatic erythrocytes (PCEs) per animal were scored for the incidence of micronucleated PCEs. The proportion of PCEs to normochromatic erythrocytes (NCEs) also was determined by counting a totoal of 1000 erythrocytes per animal.
Test substance	:	1,2-benzenedicarboxylic acid, dihexyl ester, branched and linear (disohexyl phthalate)
Conclusion	:	The test substance did not induce a statistically significant increase in bone marrow micronucleated polychromatic erythrocytes in male or female mice and was considered negative in this assay.
Reliability	:	(1) valid without restriction
Flag	:	Critical study for SIDS endpoint

05.07.2006 (7)

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

Memo : This chemical is part of the Transitional Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : Chapters 2, 3, 4 & 5

There are measured physicochemical property data available for some of the transitional phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this category. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the transitional group.

A complete health effects SIDS data set is available for dibutyl, butyl benzyl and diethylhexyl phthalate. All of these substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds in the transitional phthalate subcategory. Data on di-n hexyl phthalate (non-HPV chemical) was also included to support read-across to dihexyl, diheptyl, and diisoheptyl phthalates. The available health effects data on other HPV chemicals in this subcategory are consistent with that reported for the above reference phthalates. Thus, studies from the reference compounds (DBP, BBP, DEHP and di-n hexyl) will be used as read-across to predict the toxicity of the remaining untested members.

There is a full data set for environmental toxicity data on DBP, BBP, DHP, DEHP, and DIOP. The lower transitional phthalates (DBP, BBP) are more water soluble than higher transitional phthalates and cause acute aquatic toxicity in the 1-10 mg/L range. There is an apparent cut-off in acute toxicity at dihexyl phthalate and higher; these results are further confirmed with QSAR modeling. Both calculated and measured values for environmental toxicity endpoints predict no effects at the limit of water solubility. The dihexyl phthalate data, together with read across from DIOP to diheptyl and diisoheptyl provide sufficient test data to indicate that these phthalates have no associated acute aquatic toxicity but may show chronic toxicity. Read across from DEHP, together with QSAR modeling also confirm that diisooctyl phthalate has neither acute nor chronic aquatic toxicity.

05.07.2006

10.3 RISK ASSESSMENT